

Appendix A



## FIGURE 1 (CONT.)

	A. C.	PRABELLE			UKET	(CONI.)			
MOTA	1912	0	ASP	319	82.640	80.353	71.870	1.00	16.26
MOTA	1913	N	ALA	320	80.593	81.055	72.464	1.00	11.91
ATOM	1914	CA	ALA	320	80.102	79.758	72.914	1.00	7.79
MOTA	1915	CB	ALA	320	80.830	79.315	74.163	1.00	3.09
MOTA	1916	C	ALA	320	78.632	79.953	73.218	1.00	8.10
MOTA	1917	0	ALA	320	78.165	81.092	73.284	1.00	9.40
MOTA	1918	N	LEU	321	77.900	78.856	73.404	1.00	8.90
MOTA	1919	CA	LEU	321	76.467	78.917	73.713	1.00	6.89
MOTA	1920	CB	LEU	321	75.645	78.427	72.529	1.00	2.00
MOTA	1921	CG	LEU	321	75.538	79.283	71.268	1.00	2.00
MOTA	1922	CD1	LEU	321	75.062	78.394	70.158	1.00	4.37
ATOM	1923	CD2	LEU	321	74.589	80.461	71.444	1.00	2.00
MOTA	1924	С	LEU	321	76.121	78.088	74.947	1.00	8.16
MOTA	1925	0	LEU	321	76.665	77.008	75.1 <i>44</i>	1.00	10.39
MOTA	1926	N	ARG	322	75.258	78.618	75.804	1.00	7.97
MOTA	1927	CA	ARG	322	74.836	77.907	77.001	1.00	7.47
MOTA	1928	СВ	ARG	322	74.697	78.883	78.168	1.00	9.30
ATOM	1929	CG	ARG	322	74.550	78.23 <del>4</del>	79.535	1.00	15.10
ATOM	1930	CD	ARG	322	74.657	79.288	80.642	1.00	18.83
ATOM	1931	NE	ARG	322	74.309	78.765	81.965	1.00	18.29
ATOM	1932	CZ	ARG	322	73.750	79.488	82.932	1.00	17.03
ATOM	1933	NH1	ARG	322	73.483	80.771	82.740 84.070	1.00	18.79
ATOM	1934	NH2	ARG	322	73.411	78.921	84.078	1.00	16.70
MOTA	1935	C	ARG	322	73.486	77.329	76.602	1.00	8.75
ATOM	1936 1937	0 N	ARG VAL	322	72.535	78.071	76.373 76.455	1.00	10.16
ATOM ATOM	1937	CA	VAL	323	73.424	76.012 75.346	76.455 76.022	1.00	8.83
ATOM	1939	CB	VAL	323 323	72.209 72.523	75.346 74.365	76.023 74.871	1.00 1.00	10.03 9.77
ATOM	1939	CG1	VAL	3 <u>2</u> 3	72.323 71.306	74.363 73.549	74.507 74.507	1.00	9.77 16.85
ATOM	1941	CG2	VAL	323	71.300	75.545 75.137	74.507 73.653	1.00	7.40
ATOM	1942	C	VAL	323	72.933 71.473	74.633	77.153	1.00	13.18
ATOM	1943	Ö	VAL	323	72.053	73.803	77.853	1.00	15.89
ATOM	1944	N	GLY	324	70.196	74.969	77.327	1.00	12.40
ATOM	1945	CA	GLY	324	69.392	74.347	78.362	1.00	13.80
MOTA	1946	С	GLY	324	68.211	75.201	78.791	1.00	14.53
MOTA	1947	0	GLY	324	68.367	76.397	78.997	1.00	17.39
ATOM	1948	N	MET	325	67.026	74.613	78.901	1.00	11.83
ATOM	1949	CA	MET	325	65.868	75.368	79.341	1.00	13.08
ATOM	1950	CB	MET	325	65.201	76.124	78.186	1.00	12.41
ATOM	1951	CG	MET	325	64.150	77.118	78.678	1.00	10.52
MOTA	1952	SD	MET	325	63.227	78.025	77.440	1.00	13.36
MOTA	1953	CE	MET	325	62.495	79.307	78.488	1.00	7.16
ATOM	1954	C	MET	325	64.829	74.561	80.130	1.00	15.26
MOTA	1955	0	MET	325	64.051	73.781	79.563	1.00	15.50
ATOM	1956	N	GLY	326	64.848	74.751	81.447	1.00	15.85
ATOM	1957	CA .	GLY	326	63.899	74.093	82.323	1.00	17.08
ATOM	1958	C	GLY	326	64.165	72.651	82.677	1.00	18.22
MOTA	1959	0	GLY	326	63.270	71.957	83.148	1.00	18.82
ATOM	1960	N	CYS	327	65.401	72.206	82.515	1.00	20.56
ATOM	1961	CA	CYS	327	65.746	70.823	82.821	1.00	22.33
ATOM	1962	CB	CYS	327 327	66.443	70.194	81.622	1.00	20.50
MOTA	1963	SG	CYS	327	67.878 66.633	71.121	81.089	1.00	21.45
ATOM ATOM	1964 1965	CO	CYS CYS	327 327	66.633	70.710	84.061 84.487	1.00	24.86 26.55
ATOM .	1965	N	GLY	327 328	66.992	69.597	84.487 84.640	1.00	26.55
ATOM	1966	CA	GLY	328 328	67.007 67.846	71.859 74.867	84.619	1.00	23.64
ATOM	1967	C	GLY	3∠6 328	67.066	71.867	85.802	1.00	23.90
ATOM	1969	Ö	GLY	328	65.913	71.347 71.735	86.988 87.168	1.00 1.00	23.07
	1303	•	OL 1	JEO	UU.3 13	11.133	87.168	1.00	23.22

## FIGURE 1 (CONT.)

ATOM	1970	N	SER	329	67.706	70.528	87.822	1.00	23.68
ATOM	1971	CA	SER	329	67.077	69.925	89.000	1.00	22.19
MOTA	1972	CB	SER	329	68.150	69.406	89.964	1.00	19.55
MOTA	1973	OG	SER	329	69.028	70.440	90.356	1.00	23.14
MOTA	1974	C	SER	329	66.077	70.812	89.747	1.00	23.28
MOTA	1975	0	SER	329	64.978	70.362	90.065	1.00	25.72
MOTA	1976	N	ILE	330	66.444	72.070	89.992	1.00	22.81
MOTA	1977	CA	ILE	330	65.584	73.024	90.700	1.00	19.85
MOTA	1978	CB	ILE	330	66.410	74.017	91.589	1.00	15.67
MOTA	1979	CG2	ILE	330	66.509	73.500	93.001	1.00	18.25
ATOM	1980	CG1	ILE	330	67.795	74.289	90.994	1.00	7.11
ATOM	1981	CD1	ILE	330	67.776	74.921	89.639	1.00	5.46
ATOM	1982	C	ILE	330	64.703	73.869	89.786	1.00	20.60
ATOM	1983	Ö	ILE	330	64.225	74.923	90.201	1.00	23.53
ATOM	1984	N	IMP	331	64.425	73.400	88.579	1.00	19.32
ATOM	1985	CA	IMP	331	63.641	74.206	87.649	1.00	20.33
ATOM	1986	C	IMP	331	62.148	73.909	87.498	1.00	21.39
MOTA	1987	Ö	IMP	331	61.737	72.757	87.342	1.00	22.62
ATOM	1988	CB	IMP	331	64.310	74.200	86.277	1.00	19.26
ATOM	1989	SG	IMP	331	64.038	75.775	<b>85.516</b>	1.00	16.83
MOTA	1990	P	IMP	331	71.205	71.206	87.339	1.00	24.40
ATOM	1991	01P	IMP	331	70.381	70.028	86.885	1.00	22.40
MOTA	1992	02P	IMP	331	72.615	71.144	86.864	1.00	18.66
ATOM	1993	03P	IMP	331	71.172	71.333	88.803	1.00	19.75
ATOM	1994	O5°	IMP	331	70.688	72.534	86.798	1.00	22.96
MOTA	1995	C5*	IMP	331	71.500	73.726	87.02 <del>4</del>	1.00	14.95
ATOM	1996	C4°	IMP	331	71.156	74.601	85.831	1.00	11.32
ATOM	1997	04°	IMP	331	69.758	74.898	85.861	1.00	12.20
ATOM	1998	C3°	IMP	331	71.865	75.962	85.934	1.00	12.62
ATOM	1999	O3*	IMP	331	73.078	76.011	85.208	1.00	10.24
ATOM	2000	C2*	IMP	331	70.883	76.903	85.210	1.00	13.74
MOTA	2001	O2°	IMP	331	70.752	76.706	83.816	1.00	11.66
ATOM	2001	C1°	IMP	331	69.602	76.308	85.761	1.00	14.52
ATOM	2002	N9	IMP	331	68.832	77.205	86.612	1.00	18.13
ATOM	2003	C8	IMP	331	69.321	78.030	87.599	1.00	18.02
	2004	N7	IMP	331	68.331	78.568	88.322	1.00	16.06
ATOM ATOM	2005	C5	IMP	331	67.170	78.093	87.806	1.00	19.77
ATOM	2007	C6	IMP	331	65.799	78.289	88.156	1.00	22.26
	2007	06	IMP	331 <sub>.</sub>	65.412	78.995	89.085	1.00	17.37
ATOM ATOM	2009	N1	IMP	331	64.941	70.993 77.579	87.37 <b>4</b>	1.00	25.96
	2010	C2	IMP	331	65.296	76.706	86.299	1.00	23.29
ATOM	2010	N3	IMP	331	66.567	76.700 76.524	85.957	1.00	24.20
ATOM	2017	C4	IMP	331	67.498	70.324 77.200	86.693	1.00	21.15
ATOM				332	61.333	77.200 74.959	87.564	1.00	19.04
MOTA	2013	N	ILE	332 332	59.899	74.959 74.811	87.391	1.00	18.02
MOTA	2014	CA CB	ILE			7\$.011 75.097	88.696	1.00	16.99
ATOM	2015		ILE	332	59.071 50.423		89.793	1.00	12.90
ATOM	2016	CG2	ILE	332	59.423	74.093			14.79
MOTA	2017	CG1	ILE	332	59.283	76.525	89.191	1.00	
ATOM	2018	CD1	ILE	332	58.212	77.005	90.159	1.00	8.04 20.21
ATOM	2019	C	ILE	332	59.401	75.675 75.049	86.226	1.00	20.21
MOTA	2020	0	ILE	332	58.195	75.848 76.405	86.050	1.00	21.52
ATOM	2021	N	THR	333	60.330	76.195	85.420	1.00	20.15
ATOM	2022	CA	THR	333	59.993	77.020	84.251	1.00	19.79
MOTA	2023	CB	THR	333	61.287	77.491	83.467	1.00	20.47
ATOM	2024	OG1	THR	333	61.948	78.537	84.191	1.00	18.21
ATOM	2025	CG2	THR	333	60.949	77.996	82.058	1.00	16.88
MOTA	2026	C	THR	333	59.060	76.275	83.281	1.00	18.99
ATOM	2027	0	THR	333	58.124	76.861	82.737	1.00	19.34